SOLID MICROMECHANICS: RESEARCH AND CHALLENGES

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SOLID MICROMECHANICS: RESEARCH AND CHALLENGES

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Abstract

Micromechanics and materials are essential elements in all of the transcendent technologies that are the primary drivers of the twenty first century and in the new economy. The transcendent technologies include nanotechnology, microelectronics, information technology and biotechnology. Research tools, opportunities and challenges in mechanics and materials, including micro/nanomechanics, multiscale mechanics, microscopy, radiation scattering and other nanoscale metrologies, as well as improved engineering and design of materials are presented and discussed.

Key Words: *Atomic force microscope, biotechnology, confocal microscopy, designer materials, durability, information technology, microelectronics, nano/ micromechanics nanotechnology, multi-scale modeling, scattering metrology, simulations.*

I. INTRODUCTION

The National Science Foundation (NSF) has supported basic research in engineering and the sciences in the United States for a half century and it is expected to continue this mandate through the next century. As a consequence, the United States is likely to continue to dominate vital markets, because diligent funding of basic research does confer a preferential economic advantage (1). Concurrently over this past half century, technologies have been the major drivers of the U. S. economy, and as well, NSF has been a major supporter of these technological developments. According to the former NSF Director for Engineering, Eugene Wong, there are three *transcendental* technologies:

- Microelectronics – Moore's Law: doubling the capabilities every two years for the last 30 years; unlimited scalability; nanotechnology is essential to continue the miniaturization process and efficiency.
- Information Technology [IT] – NSF and DARPA started the Internet revolution about three decades ago; the confluence of computing and communications.
- Biotechnology – unlocking the molecular secrets of life with advanced computational tools as well as advances in biological engineering, biology, chemistry, physics, and engineering including mechanics and materials.

By promoting research and development at critical points where these technological areas intersect, NSF can foster major developments in engineering. The solid mechanics and materials engineering (M&M) communities will be well served if some specific linkages or alignments are made toward these technologies. Some thoughtful examples for the M&M communities are:

- Bio-mechanics/materials
- Thin-film mechanics/materials
- Wave Propagation/NDT
- Nano-mechanics/materials
- Simulations/modeling
- Micro-electro-mechanical systems (MEMS)
- Smart materials/structures
- Designer materials

Within the seven NIST Laboratories, research is conducted in support of U. S. industry that advances the nation's technology infrastructure and enables U. S. industry to continually improve products and services. Recent strategic planning efforts have lead to the development of four programmatic focus areas, which include nanotechnology, health care, information and knowledge management, and homeland security – very much along the transcendental technologies mentioned above. NIST will be working to provide distinct contributions to each of these focus areas within the framework of its mission. New funding will continue to be requested from the U. S. Congress in support of these focus areas. For the measurement laboratories, research will continue to be conducted in the development of measurement science and technology both in

support of and outside of these focus areas.

The Center for High Resolution Neutron Scattering, or CHRNS, is a national user facility that is jointly funded by NSF and the NIST Center for Neutron Research (NCNR). The CHRNS develops and operates state-of-the-art neutron scattering instrumentation with broad applications in materials research for use by the general scientific community. When used in combination, CHRNS instruments can provide structural information on length scales from 1 nm to approximately 10 μm, and dynamic information on energy scales from approximately 30 neV (nano electron volt) to 100 meV (micro electron volt). These ranges are the widest accessible at any neutron research center in North America. The instruments are used by university, government and industrial researchers in materials science, chemistry, biology and condensed matter physics to investigate materials such as polymers, metals, ceramics, magnetic materials, porous media, fluids and gels, and biological molecules. Proposals for use of the CHRNS facilities are considered on the basis of scientific merit or technological importance. For additional information, please visit
http://rrdjazz.nist.gov/programs/CHRNS/.

II. MICRO/NANOTECHNOLOGY

II.1 MICRO/NANOMECHANICS WORKSHOP

Initiated by the senior author [K. P. Chong], with the organization and help of researchers from Brown [K. S. Kim, et al], Stanford, Princeton and other universities, a NSF Workshop on Nano- and Micro-Mechanics of Solids for Emerging Science and Technology was held at Stanford in October 1999. The following is extracted from the Workshop Executive Summary. Recent developments in science have advanced capabilities to fabricate and control material systems on the scale of nanometers, bringing problems of material behavior on the nanometer scale into the domain of engineering. Immediate applications of nanostructures and nano-devices include quantum electronic devices, bio-surgical instruments, micro-electrical sensors, functionally graded materials, and many others with great promise for commercialization. The branch of mechanics research in this emerging field can be termed nano- and micro-mechanics of materials, highly cross-disciplinary in character. A subset of these, which is both scientifically rich and technologically significant, has mechanics of solids as a distinct and unifying theme. The presentations at the workshop and the open discussion precipitated by them revealed the emergence of a range of interesting lines of investigation built around mechanics concepts that have potential relevance to microelectronics, information technology, bio-technology and other branches of nanotechnology. It was also revealed, however, that the study of complex behavior of materials on the nanometer scale is in its infancy. More basic research that is well coordinated and that capitalizes on progress being made in other disciplines is needed if this potential for impact is to be realized.

Recognizing that this area of nanotechnology is in its infancy, substantial basic research is needed to establish an engineering science base. Such a commitment to nano- and micro-mechanics will lead to a strong foundation of understanding and confidence underlying this technology based on capabilities in modeling and experiment embodying a high degree of rigor. The instruments and techniques available for experimental micro- and nano-mechanics are depicted in Fig. 1, courtesy of K. S. Kim of Brown University.

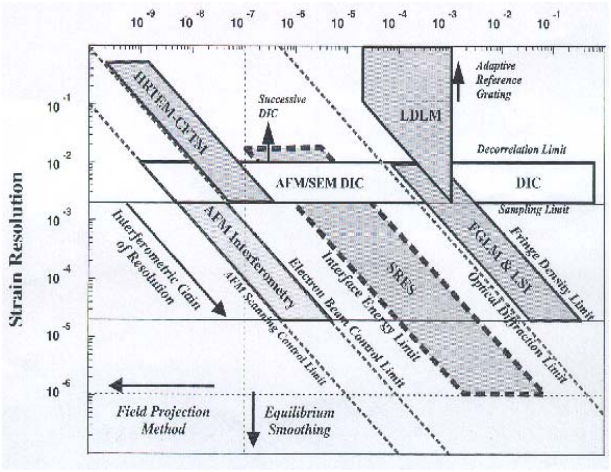


Figure 1. Instruments and techniques for experimental micro and nano mechanics (courtesy of K. S. Kim of Brown University) where

HRTEM High Resolution Transmission Electron Microscopy
SRES Surface Roughness Evolution Spectroscopy
CFTM Computational Fourier Transform Moire
FGLM Fine Grating Laser Moiré
AFM Atomic Force Microscopy
LSI Laser Speckle Interferometry
SEM Scanning Electron Microscopy
DIC Digital Image Correlation
LDLM Large Deformation Laser Moire

The potential of various concepts in nanotechnology will be enhanced, in particular, by

exploring the nano- and micro-mechanics of coupled phenomena and of multi-scale phenomena. Examples of coupled phenomena discussed in this workshop include modification of quantum states of materials caused by mechanical strains, ferroelectric transformations induced by electric field and mechanical stresses, chemical reaction processes biased by mechanical stresses, and changes of bio-molecular conformality of proteins caused by environmental mechanical strain rates. Multi-scale phenomena arise in situations where properties of materials to be exploited in applications at a certain size scale are controlled by physical processes occurring on a size scale that is orders of magnitude smaller. Important problems of this kind arise, for example, in thermo-mechanical behavior of thin-film nanostructures, evolution of surface and bulk nanostructures caused by various material defects, nanoindentation, nanotribological responses of solids, and failure processes of MEMS structures. Details of this workshop report can be found by visiting http://en732c.engin.brown.edu/nsfreport.html.

II.2 NANOSCALE SCIENCE AND ENGINEERING INITIATIVES

Coordinated by M. Roco (2), NSF recently announced a second year program (3) (see: www.nsf.gov) on collaborative research in the area of nanoscale science and engineering [NSE]. This program is aimed at supporting high risk/high reward, long-term nanoscale science and engineering research leading to potential breakthroughs in areas such as materials and manufacturing, nanoelectronics, medicine and healthcare, environment and energy, chemical and pharmaceutical industries, biotechnology and agriculture, computation and information technology, improving human performance, and national security. It also addresses the development of a skilled workforce in this area as well as the ethical, legal and social implications of future nanotechnology. It is part of the interagency National Nanotechnology Initiative [NNI]. Details of the NNI and the NSE initiative are available on the web at http://www.nsf.gov/nano or http://nano.gov.

The NSE competition will support Nanoscale Interdisciplinary Research Teams [NIRT] and Nanoscale Exploratory Research [NER]. Nanoscale Science and Engineering Centers [NSEC] awarded in the first year [FY 2001] competition will be funded on a continuing basis. In addition, individual investigator research in nanoscale science and engineering will continue to be supported in the relevant NSF Programs and Divisions outside of this initiative. This NSE initiative focuses on seven high risk/high reward research areas, where special opportunities exist for fundamental studies in synthesis, processing, and utilization of nanoscale science and engineering. The seven areas are:

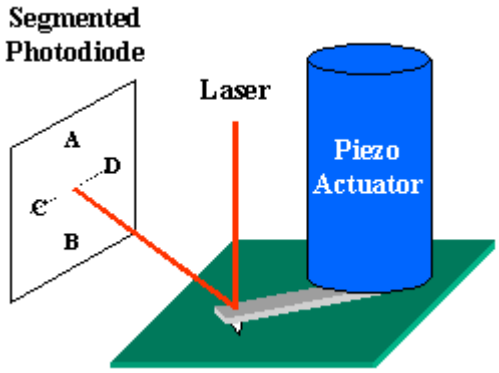
- Biosystems at the nanoscale
- Nanoscale structures, novel phenomena, and quantum control
- Device and system architecture
- Nanoscale processes in the environment
- Multi-scale, multi-phenomena theory, modeling and simulation at the nanoscale
- Manufacturing processes at the nanoscale
- Societal and educational implications of scientific and technological advances on the nanoscale

The National Nanotechnology Initiative started in 2000 ensures that investments in this area are made in a coordinated and timely manner (including participating federal agencies – NSF, DOD, DOE, DOC [including NIST], NIH, DOS, DOT, NASA, EPA and others) and will accelerate the pace of revolutionary discoveries now occurring. Current request of Federal agencies on NNI is $519 million. The NSF share of the budget is $199 million [on NSE, part of NNI].

II.3 MICROSCOPY

In atomic force microscopy [AFM], a probe consisting of a sharp tip (nominal tip radius on the order of 10 nm) located near the end of a cantilever beam is raster scanned across the sample surface using piezoelectric scanners. Changes in the tip-sample interaction are often monitored using an optical lever detection system, in which a laser beam is reflected off of the cantilever and onto a position-sensitive photodiode. During scanning, a particular operating parameter is maintained at a constant level, and images are generated through a feedback loop between the optical detection system and the piezoelectric scanners. A schematic illustration of a scanning stylus atomic force microscope is shown in Figure 2a. In this design, the probe tip is scanned above a stationary sample, while in a scanning sample design, the sample is scanned below a fixed probe tip. Operationally, little difference exists between these two designs, because the relative motion of the tip to the sample is used to generate

topographic images. Applications of AFM and other types of scanning probe microscopy continue to grow rapidly in number and include biological materials (e.g., studying DNA structure), polymeric materials (e.g., studying morphology, mechanical response, and thermal transitions), and semiconductors (e.g., detecting defects). In particular, AFM can be utilized to evaluate the surface quality of products such as paint and coating systems, contact lenses, optical components (mirrors, beamsplitters, etc.), and semiconductor wafers after various cleaning, etching, or other manufacturing processes.



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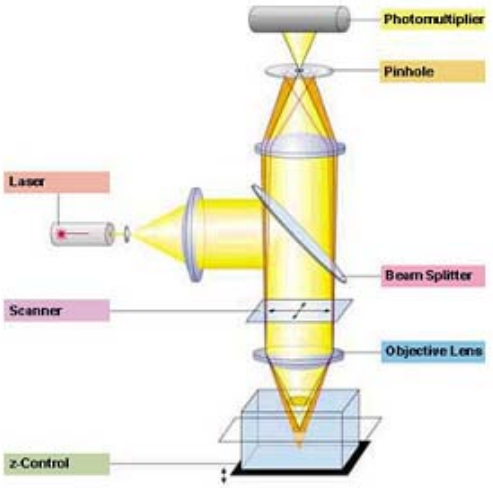
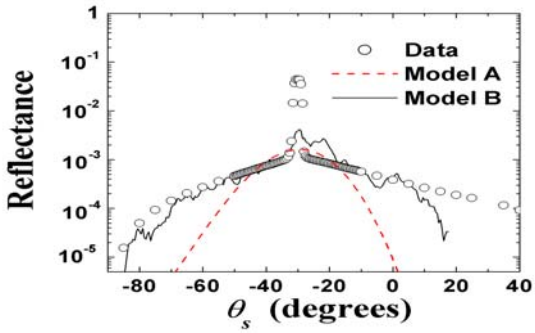


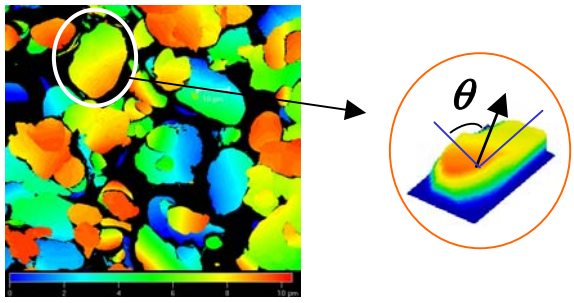
(b)

Figure 2. Schematic illustrations of (a) a scanning-probe atomic force microscope (AFM) and (b) a laser-scanning confocal microscope (LSCM).

Laser scanning confocal microscopy (LSCM) is a non-destructive, powerful tool for characterizing the microstructure of polymeric and biological materials. In Fig. 2b, the confocal principle is illustrated. A LSCM uses coherent incident light and collects reflected or scattered light exclusively from a single plane, rejecting light out of the focal plane. The laser scanning confocal microscope scans the sample sequentially point by point and line by line and assembles the pixel information into one image. Optical slices of the specimen are thus created with high contrast and high resolution in x, y and z directions. By moving the focal plane systematically, a series of optical slices are created that can be used to construct a three-dimensional image stack that can be digitally processed. The wavelength, numerical aperture (N.A.) of the objective, and the size of the collecting pinhole in front of the detector determine the resolution in the thickness or axial direction (4). Microstructure information obtained from LSCM results can be used, for example, to model scattering properties of coating materials, which can then be compared to scattering measurements using light scattering (5). Fig. 3a shows the comparison of the measured calculated reflectance data from the corresponding confocal image (3D topographic data (Fig. 3b) and flake orientation data (Fig. 3c). Here, model A using a Gaussian distribution to represent the measured flake orientation distribution as a input while Model B using a topographic map (including local surface roughness and orientation) of the flakes as input to a ray scattering model to calculate the optical reflectance of each coating. Details of the theory and discussion can be found in Ref. 5.



(a)

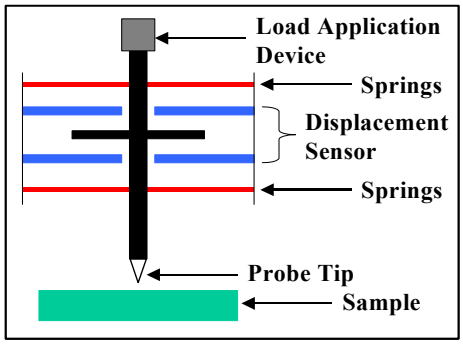


(b) (c)

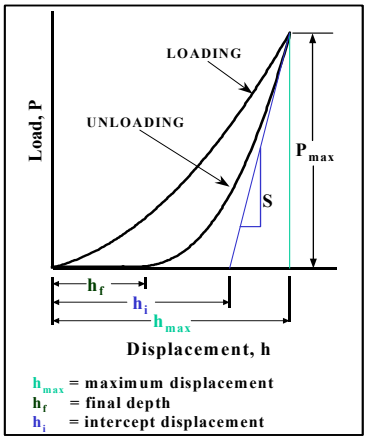
Figure 3. (a) Comparison of the *measured and calculated reflectance data, (b) the corresponding confocal 3D topographic data, and (c) individual flake orientation.*

II.4 NANOMECHANICS

Measurements of mechanical behavior of very small volumes of material have been enabled by the development of instruments that can sense and apply very small forces and displacements, including AFMs and nanoindenters. These devices are often capable of producing contact areas and penetration depths characterized by nanometer dimensions while also providing lateral motion capabilities for studying tribological behavior. One objective of using these devices is to provide methods for characterizing mechanical response of material systems with nanoscale spatial resolution. Such measurements can be a key to understanding technologically important material systems, including those used in magnetic storage, microelectronic and telecommunication devices. Further, these types of measurements are important in support of nanotechnology developments, e.g., nanoelectronic devices and nanostructured materials such as ultra-thin films and nanocomposites.



(a)



(b)

Figure 4. Schematic illustrations of (a) a nanoindentation system and (b) load-displacement or load-penetration data produced from a nanoindentation measurement, including key characteristics.

Nanoindentation via the AFM is performed in a non-scanning mode, termed force mode, in which the AFM probe is moved toward the sample surface, pushed into the surface, and then lifted back off of the surface (see Fig. 2a). A force-displacement curve is produced from which a force-penetration curve related to the nanoindentation process can be determined. The force applied is related to the deflection (bending) of the cantilever beam through the cantilever spring constant, and the penetration into the material is the difference between the overall vertical displacement of the cantilever and the probe tip displacement related to cantilever bending, which must be calibrated. For nanoindentation devices, shown schematically in Fig. 4a, the application of force and the measurement of displacement are often done using electromagnetic or electrostatic transducers. System compliance must be calibrated to eliminate displacement of the load frame, such that force-penetration curves are produced (see Fig. 4b). Typically, the unloading data is assumed to be primarily elastic recovery of the material and is often analyzed using a power law curve fit of the form:

$$P = \alpha\left(h - h_f\right)^m$$

where P is force, h is penetration, h_f is the penetration after unloading, and α and m are curve fitting parameters. The slope, dP/dh, taken at the point of maximum load, P_{max}, and maximum displacement, h_{max}, is the contact stiffness, S, which is used to first determine the contact depth, h_c,

$$h_c = h_{\max} - \frac{\varepsilon P_{\max}}{S}$$

here ε is a parameter related to the contact geometry, and subsequently to calculate elastic modulus,

$$E_r = \frac{\sqrt{\pi}}{2\beta}\frac{S}{\sqrt{A}}$$

where A is the contact area, which is calculated from knowledge of the tip shape and h_c, β is a parameter related to tip geometry, and E_r is the reduced or effective modulus, which is related to values of modulus and Poisson's ratio for the sample (E_s and

ν_s) and indentation tip (E_i and ν_i):

$$\frac{1}{E_r} = \frac{\left(1-\nu_s^2\right)}{E_s} + \frac{\left(1-\nu_i^2\right)}{E_i}$$

Indentation hardness, H, can also be calculated as the maximum load, P_{max}, divided by the contact area, A.

Recent advances in instrumentation have focused on improvements in sensitivity, the addition of testing capabilities, and the integration of force measurements and imaging. For nanoindentation devices, improvements in sensitivity have been made by adding dynamic capabilities to these systems, which previously have operated only in a quasi-static mode. Often, a dynamic signal with a displacement amplitude on the order of 1 nm is superimposed over a quasi-static loading history. This type of technique allows hundreds of measurements of elastic modulus and hardness to be calculated as opposed to a single measurement from a quasi-static indentation test. Also, dynamic behavior of the materials, e.g., storage and loss characteristics, can be studied, often over a range of frequencies, similar to dynamic mechanical analysis. Other additional capabilities include lateral motion and lateral force measurement capabilities for tribological studies, including scratch testing, and improvements to the control systems that allow for automated testing using a variety of user-specified loading histories.

Integration of force measurements and imaging capabilities has been made in both AFM systems and in hybrid AFM-nanoindentation devices. AFM images are now produced routinely using particular aspects of the tip-sample force interactions. Each pixel in the image represents a position on the sample at which a force-distance curve was measured. The image can then be set up to indicate changes in local tip-sample adhesion or sample stiffness, for example. However, mechanical property measurements associated with SPM systems have significant uncertainties in the probe spring constant and tip shape, which typically render them useful only as qualitative information (6). More quantitative measures of tip-sample forces can be achieved for systems that employ force transducers in combination with scanning capabilities similar to AFM. Examples of such systems include the interfacial force microscope or IFM developed at Sandia National Laboratories (7) and a commercial force transducer that interfaces with many commercial AFM systems (8,9).

While advances in instrumentation continue, questions remain regarding uncertainties associated with measurement and calibration techniques. Current research at NIST is focused on measurement systems for calibrating micro-Newton forces. Questions regarding the use of reference materials for calibrating load-frame compliance and tip shape as well as other analysis and procedural issues persist with regard to nanoindentation measurements that must be addressed. For example, recent studies, including an interlaboratory comparison (10), have shown the calibration results to have poor reproducibility and large uncertainties.

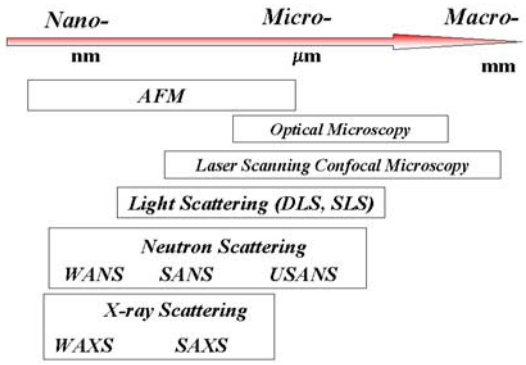


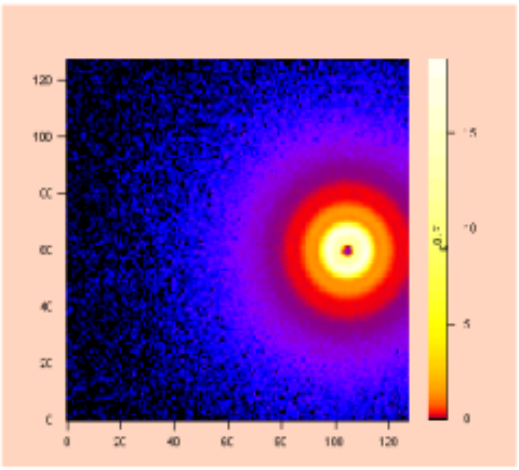
Figure 5. Capabilities of different microscopy and scattering techniques.

II.5 SCATTERING METROLOGY

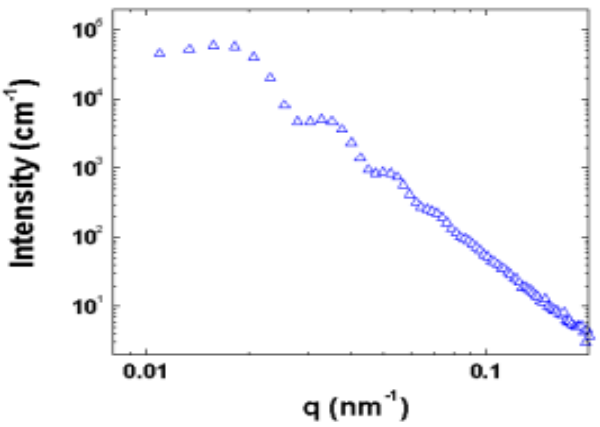
Scattering metrology is widely used for characterizing nano-/micro-domains and nano-structural features of polymers and other materials, and is a complimentary technique to microscopy tools. Many forms of radiation can be used for scattering purposes: x-rays, neutron, laser light, electrons, etc. Each has different characteristics and is used for different purposes. In general, the principle and operation of measurements is similar. However, the microstructural information generated could be different due to the different interactions between the scattering source and the materials. For example, neutron scattering is sensitive to inhomogeneities in density of nuclei in the materials, while light or x-ray scattering is sensitive to inhomogeneities in the refractive index or electron density in the materials. In this paper, we will only describe the neutron scattering method.

In Fig. 5 the relative measurable length scale using different scattering metrology and microscopy techniques are shown. The small-angle neutron and

x-ray scattering methods (SANS, SAXS) are useful for polymer research (or condense matter research in general) because they probe size scales from angstrom-level to micron-level. With recently developed Ultra-SANS (USANS) instruments, the length scales using neutron scattering method can be extended to 10 μm (11). Static light scattering (SLS) complements these techniques by focusing on the micron length scale. Dynamic light scattering (DLS) can be used for measuring diffusive motion and particle sizing in complex fluid systems from 1 nm to 5 μm. Other methods such as wide-angle neutron and x-ray scattering (WANS, WAXS) probe very local (atomic) structure on the order of a few nanometers.



(a)



(b)

Figure 6. (a) A two-dimensional scattering image, and (b) the corresponding absolute scattering intensity curve as a function of the scattering wave vector q, for a polymeric system with a well-ordered structure.

The NIST Center for Neutron Research (NCNR), which maintains the leading neutron scattering facility in the U. S., offers advanced measurement capabilities for use by all qualified applicants. Information on instrumental description may be obtained at the NCNR website [http://www.ncnr.nist.gov/]. Many of its instruments rely on intense neutron beams produced by a liquid hydrogen cold neutron source (12). The small angle neutron scattering (SANS) instrument is a powerful tool for characterizing nano-/ micro-domains and nanostructures of various polymeric systems as well as particles or fillers in solution or in a polymer matrix.

In Fig. 6, SANS results obtained from nano-size fillers (for example: inorganic pigment) in a polymer matrix are shown. After standard calibrations and taking into account the sample transmission and film thickness, two-dimensional scattering images (see Fig. 5a) are averaged azimuthally to produce a one-dimensional absolute scattering intensity curve (see Fig. 5b) as a function of the scattering wave vector q. ($q = 4\pi\sin(\theta/2)/\lambda$, where θ is the scattering angle and λ is the wavelength). In this case, the filler has a higher neutron scattering coefficient than the polymer matrix, and the neutron scattering intensity is proportional, to the first order, to differences in the local filler concentrations within the sample. Typically the scattering intensity, I(q), can be modeled as following:

$$I(q) = I_o\, P(q)\, S(q),$$

where $P(q)$ is the form factor, and $S(q)$ is the structure (13). The wavelength independent part of the equation: I_o is proportional to the scattering amplitude (scattering contrast between the fillers and the polymer matrix), the number density, and the volume of the fillers. The form factor $P(q)$ comes from the intramolecular interferences and is characteristic of the size and shape of the particles. For a particle with well-defined shape, such as a spherical particle with uniform scattering density (see example of Fig. 6b) or a spherical particle with a core-shell structure, the form factor $P(q)$ can be calculated, and the size of the particles can be determined.

The structure factor S(q) is related to the correlation function describing the radial distribution function between particles or micro-domains. The intra-particle, intra-domain interaction parameters can be also determined by fitting S(q) to a theoretical modeling. A peak in the scattering profile at a scattering wave vector q indicates the

existence of micro-domains with a characteristic average length $d = 2\pi/q$. The microstructure/morphology information, such as the dimension of ordered domains or the correlation length of concentration fluctuations, can be determined from the intensity profile.

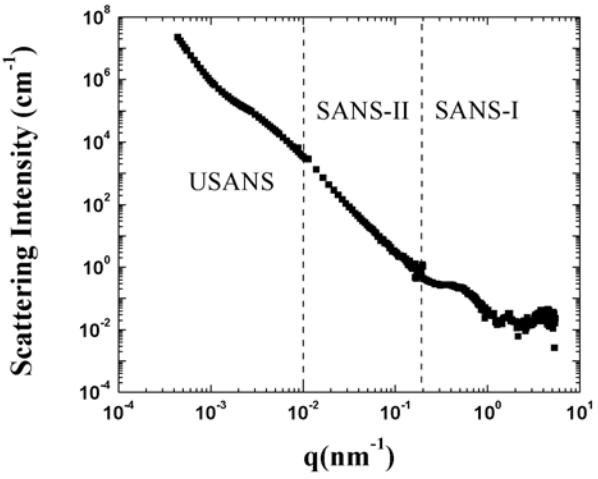


Figure 7: Scattering Intensity for a complex system of 5 % Cloisite 15A clay platelet in a matrix of PE-EVA (polyethylene -ethyl vinyl acetate) using various neutron scattering techniques.

For complex systems, combinations of various scattering techniques are often used to investigate the microstructure / morphology at various length scales. Fig. 6 shows the scattering profile for a complex system of 5 % Cloisite 15A (organically modified montmorillonites) clay platelet in a matrix of PE-EVA (polyethylene-ethyl vinyl acetate) using various neutron scattering techniques as indicated in three regions. The three regions present:

- *SANS-I*: using regular 30m SANS operating configurations at NCNR, maximum probing length ~ 200 nm.

- *SANS-II*: using the SANS instrument with a special focusing neutron optics-device (14) to achieve the probing length to the order of 500 nm.

- *USANS*: using a perfect crystal diffractometer (PCD) for ultra-high resolution small-angle neutron scattering (USANS) measurements at the thermal neutron beam port in NCNR (11). The probing length covering over about two orders of magnitude, from ~10^2 nm to 10^4 nm.

As shown in Fig. 6, the overall accessible q range is more than four decades and probing structure in materials is over four orders of magnitude, from ~1 nm to 10^4 nm. Combined measurements on these instruments will enable hierarchical and highly anisotropic microstructures in materials, for example in fiber or clay impregnated nanocomposites (data shown in Fig. 6, Ref 15.), to be more fully characterized.

II.6 DIFFRACTION AND ENGINEERING APPLICATIONS

Diffraction techniques (neutron and x-ray) have been widely used for crystallographic characterization of materials. Neutrons have a number of advantage and disadvantages compared to x-ray, for example: neutron provide much better sensitivity to establishing the location of lighter atoms in the unit cell. Neutron are far more penetrating than x-ray, allowing the bulk of a sample to be probed in contrast to x-ray experiment that are usually surface–sensitive. Referred to "*Materials Research With Neutrons at NIST*" by Cappelletti, at el. (12) for detailed descriptions of the material research applications and neutron diffraction instrumentation in NCNR.

In addition to the application of crystallographic characterization, neutron diffraction has been applied to measure the depth profiling of residual strain. (http://rrdjazz.nist.gov/instruments/darts/) Neutron diffraction measurements at the NCNR that have contributed new insights into how Ultrasonic Impact Treatment actually affects residual stresses in the weld region around a full-scale cover plate for a steel girder (16). (see example: Fig. 8) Current research projects at NCNR on residual stress and texture measurements of different materials and systems, such as railroad rails, plasma sprayed coatings, and etc., will definitely provide technical insights for improving mechanical and materials properties.

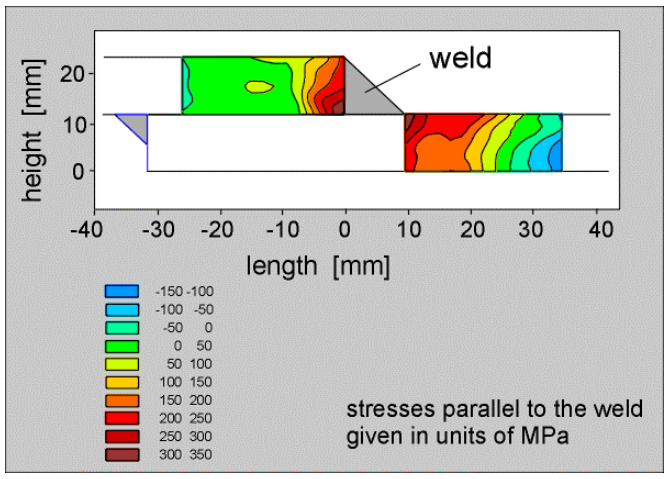


Figure 8: Internal residual stresses due to welding measured by the neutron diffraction method.

III. MODELING AND SIMULATION

The initiative *Engineering Sciences for Modeling and Simulation-Based Life-Cycle Engineering* (Program Announcement NSF 99-56) is a three-year collaborative research program by NSF and the Sandia National Laboratories [Sandia] focusing on advancing the fundamental knowledge needed to support advanced computer simulations. This collaborative initiative capitalizes on the missions of both organizations. NSF's mission is to advance the fundamental science and engineering base of the United States. Sandia has the responsibility to provide solutions to a wide range of engineering problems pertinent to national security and other national issues. It is moving toward engineering processes in which decisions are based heavily on computational simulations including meshless methods in moving boundary problems (17); thus, capitalizing on the available high performance computing platforms. This initiative has sought modeling and simulation advances in key engineering focus areas such as thermal sciences, mechanics and design.

The NSF Civil and Mechanical Systems [CMS] Division developed an initiative on *Model-based Simulation* (MBS), see NSF 00-26. Model-based simulation is a process that integrates physical test equipment with system simulation software in a virtual test environment aimed at dramatically reducing product development time and cost. This initiative will impact many civil/mechanical areas: "structural, geotechnicial, materials, mechanics, surface science, and natural hazards (e.g., earthquake, wind, tsunami, flooding and land-slides)." MBS would involve "combining numerical methods such as finite element and finite difference methods, together with statistical methods and reliability, heuristics, stochastic processes, etc., all combined using super-computer systems to enable simulations, visualizations, and virtual testing." Expected results could be less physical testing, or at best, better strategically planned physical testing in the conduct of R&D. Examples of the use of MBS in research, design and development exist in the atmospheric sciences, biological sciences, and the aerospace, automotive and defense industries. The manufacturing of the prototype Boeing 777 aircraft, for example, was based on computer-aided design and simulation, cutting costs and shortening production time significantly.

The NIST Center for Theoretical and Computational Materials Science (CTCMS) was established to investigate important problems in materials theory and modeling with novel computational approaches. The Center creates opportunities for collaboration where CTCMS can make a positive difference by virtue of its structure, focus, and people. It develops powerful new tools for materials theory and modeling and accelerates their integration into industrial research. The current technical focus areas include: modeling microstructure and mechanical response using object-oriented finite element analysis, micromagnetic modeling, nanofilled polymer melts, deformation of metals…etc. Detailed information can be found on the center web site at http://www.ctcms.nist.gov/programs. In addition to the current projects, the CTCMS is continuously soliciting proposals for workshops on materials theory and modeling, short-term and long-term visiting fellowship, guest researcher, and NRC postdoctoral positions, and creative and ambitious new projects in materials theory and modeling.

In the future one should expect the continued introduction of bold innovative research initiatives related to important national agenda issues such as the environment, civil and mechanical infrastructure, the service industry and the business enterprises.

III. CHALLENGES

Mechanics and materials engineering are really two sides of a coin, closely integrated and related. For the last decade this cooperative effort of the M&M Program has resulted in better understanding and design of materials and structures across all physical scales, even though the seamless and realistic modeling of different scales from the nano-level to the system integration-level (Fig. 9) is not yet attainable. In the past, engineers and material scientists have been involved extensively with the characterization of given materials. With the availability of advanced computing and new developments in material science, researchers can now characterize processes and design and manufacture materials with desirable performance and properties. One of the challenges is to model short-term micro-scale material behavior, through meso-scale and macro-scale behavior into long-term structural systems performance. Accelerated tests to simulate various environmental forces and impacts are needed (18). Supercomputers and/or workstations used in parallel are useful tools to solve this scaling problem by taking into account the

large number of variables and unknowns to project micro-behavior into infrastructure systems performance, and to model or extrapolate short term test results into long term life-cycle behavior (18, 19). Twenty-four awards were made totaling $7 million. A grantees' workshop was held recently in Berkeley and a book of proceedings has been published (20).

Many current NIST projects are focused on multidisciplinary and multi-scale problems, including in the areas of materials and mechanics. One successful program in the NIST Building and Fire Research Laboratory is the Service Life Prediction or SLP program, which includes partnerships with industry and other U. S. Federal Agencies. The methodology that is being used to reduce the time to generate these durability performance histories to months instead of years is called reliability theory and life testing analysis. This methodology has had a long and successful history of application in predicting the service life of electronic, aerospace, nuclear, and medical products, and is currently being applied in five different, but highly overlapping, project areas including: 1) appearance (the primary measure of durability for a coating system), 2) coatings and pigments, 3) composites, 4) polymeric interphases, and 5) sealants. This research effort includes implementing and developing use-inspired scientific and technical advances in methodologies and metrologies for improving and advancing the appearance, service life, and performance of polymeric construction materials. Included in this effort is an integration of materials science, metrology from nanoscale though macroscale including nanomechanics, high-throughput testing and analysis, and information management.

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MATERIALS		**STRUCTURES**	**INFRASTRUCTURE**	
nano-level (10^{-9})	**micro-level (10^{-6})**	**meso-level (10^{-3})**	**macro-level (10^{+0})**	**systems-level (10^{+3}) m**
Molecular Scale	***Microns***	***Meters***		***Up to Km Scale***
***nano-mechanics**	***micro-mechanics**	***meso-mechanics**	***beams**	***bridge systems**
***self-assembly**	***micro-structures**	***interfacial-structures**	***columns**	*** lifelines**
***nanofabrication**	***smart materials**	***composites**	***plates**	***airplanes**

Figure 6. Physical scales in materials and structural systems (from Ref. 17)